## Membrane Structure II

**2658-Pos Board B644**

**Data Compression for Molecular Simulations**

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Storage of large molecular dynamics (MD) simulation measurements in standard databases is a challenging task. The requirements on disk space, input/output (I/O) and data transfer bandwidth are excessively high due to the large volume, possibly terabytes or petabytes, of data generated. Storage of data in compressed form has been a popular approach to address such issues. In this paper, we present a lossy compression framework that yields significant performance gain by combining the strength of the principal component analysis (PCA) and discrete cosine transform (DCT).

In our framework, the MD data are first transformed, using PCA, from the generic 3-D coordinate space to another 3-D eigen space, with the dimensions sorted in decreasing importance levels in capturing the variance of the atoms's movements. In the eigen space, the DCT is applied to each dimension to achieve lossy compression across a number of consecutive atom frames. The combination of the PCA and DCT ensures that our framework is able to (1) achieve balanced compression across 3-D coordinate space, (2) realize dynamic error control and avoid the propagation of the compression errors and data corruptions; and (3) ensure random access to any portion of the data without fully decompressing the whole data file. Experimental results using real simulation data show that the data storage space requirement is reduced by a large magnitude while achieving a compression ratio of about 13. Errors comparable to the existing techniques are achieved with minimal computational overhead.

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**Refining and Testing CHARMM Lipid Parameters for Biologically Important Membranes**

Joseph B. Lim, **Jeffery B. Klauda**.

Biological membranes form a barrier to protect the cell from its environment and consist of a wide variety of lipids. A recent modification to the CHARMM lipid force filed, CHARMM36 (C36), resulted in significant improvements in deuterium order parameters (SCD), water hydration, and area compressiblities. Moreover, C36 simulations resulted in excellent surface areas per lipid compared to experiment with NPT molecular dynamics (MD). We have extended this force field to aliphatic chain branched lipids, which exists in many bacterial membranes. MD simulations of DPhPC agree with experimental form factors and suggest that current lipid force field parameters are valid for these branched chain lipids. Branching leads to an increase in average surface areas per lipid, area elastic moduli and lipid axial relaxation times. However, MD simulations of mixed bilayers with cholesterol and polyunsaturated lipids suggest that the atomistic force field describing these lipids requires modification (improper sterol orientation and head-to-head group spacings). MD simulations on decalin resulted in a heat of vaporization that is 10 kJ/mol lower than experiment, but modifications to the Lennard-Jones parameters of cholesterol yielded near perfect agreement with experiment. Simulations with these parameters were in excellent agreement with experimental SCDs for the DMPC acyl chain and SCDs for ring and chain positions on cholesterol. Moreover, these simulations agree favorably with experimental form factors of DMPC-cholesterol bilayers. However, simulations with a polyunsaturated lipid, DAPC, and cholesterol still resulted in the abovementioned inaccuracies. Since the thickness of these polyunsaturated bilayers was too large by ~8 Å, high-level quantum mechanical (QM) calculations were used for dihedrals adjacent to the double bonds. It was found that the previous force field restricted the conformational flexibility and MD simulations are underway to test the QM-based potentials accuracy compared to experimental diffraction studies.

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**In Silico Model Escherichia Coli Membranes: Simulating a Lipid with a Cyclopropane Ring**

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Bacterial membranes are composed mostly of lipids with phosphoethanolamine (PE) and phosphoglycerol (PG) head groups and a variety of fatty acid chains. A defining characteristic of bacterial membranes is the presence of lipids with a cyclic-containing chain. To our knowledge, a phospholipid with such a chain has never been studied in a molecular dynamics simulation. Thus, novel force field parameters to describe a cyclopropane moiety were developed using parameters from the CHARMM36 (C36) general force field as a basis and high-level quantum mechanical energies. Two simple membranes and one complex membrane for use as realistic model *Escherichia coli* (*E. coli*) cytoplasmic membranes were designed for future work with secondary active transporters expressed in *E. coli*. Compositions of the membranes were based on several different experimental methods using an *E. coli* K12 strain grown on Luria broth. One simple membrane consisted of 85 % PE 18:1/16:0 (POPE) and 15 % PG 18:1/16:0(POPG), and the other of only PE cy17:0/16:0 (PMPE). The complex membrane consisted of six different phospholipids, the most prevalent being the cyclic-containing lipid, PMPE. NPT simulations were carried out at 310 K for 50 ns using the C36 lipid force field and the developed cyclopropane moiety force field for each membrane. NMR deuterium order parameters ($S_{CD}$), density profiles, and diffusion constants are compared with experiment. The model membranes will provide a basis to study membrane bound proteins or other bound molecules expressed in *E. coli* with realistic molecular dynamic simulations.

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**Structure and Bending Rigidity of SOPC, SOPC-Cholesterol, and SOPC-LWYIK Bilayers: A Comparison of Molecular Dynamics and X-Ray Scattering Results**

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Using molecular dynamics simulations, we investigate the structure and material properties for SOPC, SOPC-Cholesterol, and SOPC-LWYIK bilayer systems. Using a novel algorithm, we solve for electron density profiles from large undulating bilayer systems and compare the resulting form factors to low angle x-ray scattering (LAXS) data. Using undulation spectral analysis we solve for $k_C$, the bending modulus, from both united-atom and coarse-grained molecular dynamics simulations and compare these findings to published experimental results (Greenwood, A. I. et al. 2008). For SOPC-LWYIK, we present a multi-faceted approach that explores starting configurations, such as potential of mean force (PMF), reverse coarse-graining as well as brute force molecular dynamics as treatments to facilitate equilibration of the system.

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**Sugar-Membrane Interactions: An All-Atom Replica Exchange Molecular Dynamics Study of a Virulent Factor from tb**

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Tuberculosis, one of the fatal diseases, is caused by Mycobacterium tuberculosis (M. tb.). The most virulence factor of M. tb. is lipoarabinomannan (LAM), which is a glycolipid present in pathogen's cell envelope. LAM affects the host immune response by interfering host cell-signaling. Specifically, the mannose-cap (di-mannose) portion of LAM is responsible for inhibiting fusion of phagosome with lysosomes known as P-L fusion, which diminishes the ability of the host macrophages to kill the invading M. tb. The physical chemistry of the effects of mannose on lipid membrane has not been well characterized. Here, we conduct constant pressure all-atom replica exchange molecular dynamics simulations using CHARMM c36 force field to understand the interaction between di-mannose and membrane. Two types of lipid bilayers are considered: 1-palmitoyl-2-oleoyl-sn-phosphatidylcholine (POPC) and 1,2-dioleoyl-sn-phosphatidylcholine (DOPC). Through our simulations we are seeking answers to questions such as whether the mannose cap is preferred in solution or lipid-water interface and how does the mannose cap affect the membrane fluidity and other properties such as area per lipid and bilayer thickness. We present results that are based on two different di-mannose concentrations.

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**Molecular Modeling of Membrane Interactions with Trehalose - A Molecular View on the Water Replacement Hypothesis**

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Lipid Bilayers are the fundamental scaffold representing cell membranes. In order to understand cell interactions with the environment we need to understand lipid bilayer interactions. Here we are presenting effects of the low molecular weight sugar trehalose on lipid bilayers in the hydrated and dry state. We show by detailed simulations that trehalose can significantly alleviate dehydration injury in bilayer stacks as well as in single bilayers. To simulate the latter we needed to develop a way to suppress the interactions of bilayers under periodic boundary conditions. A main effect is the change of the hydrogen bonding network and the membrane electric potential under dehydration with and without sugars. The state of the membrane under dehydration with sugars is in area per molecule (fluidity) similar to a free bilayer. However, structural properties are significantly altered.